NOMAD
NOVEL MATERIALS DISCOVERY

MAX-PLANCK-GESELLSCHAFT

Data-driven cartography of materials properties

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Workshop on Crystal Structure Prediction:
Exploring the Mendeleev Table as a Palette to Design New Materials
ICTP, Trieste, 13-18 January 2019

Data-driven materials science: the big picture

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- Design of new materials:
  preparation, synthesis, and characterization is complex and costly
- About 240000 *inorganic* materials are known to exist (Springer Materials)
- Basic properties determined for very few of them
- Number of possible materials: practically infinite

⇨ New materials with superior properties exist but not yet known

- Data-analytics tools will help to identify trends and anomalies in data and guide discovery of new materials

We have a dream

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From the **periodic table of the elements** to a **chart of materials**

Reihen	Gruppe I. — R^2O	Gruppe II. — RO	Gruppe III. — R^2O^3	Gruppe IV. RH^4 RO^2	Gruppe V. RH^3 R^2O^5	Gruppe VI. RH^2 RO^3	Gruppe VII. RH R^2O^7	Gruppe VIII. — RO^4
1	H=1							
2	Li=7	Be=9.4	B=11	C=12	N=14	O=16	F=19	
3	Na=23	Mg=24	Al=27.3	Si=28	P=31	S=32	Cl=35.5	
4	K=39	Ca=40	—=44	Ti=48	V=51	Cr=52	Mn=55	Fe=56, Co=59, Ni=59, Cu=63.
5	(Cu=63)	Zn=65	—=68	—=72	As=75	Se=78	Br=80	
6	Rb=85	Sr=87	?Yt=88	Zr=90	Nb=94	Mo=96	—=100	Ru=104, Rh=104, Pd=106, Ag=108.
7	(Ag=108)	C			22	Te=125	J=127	
8	Cs=133	Ba=137	?Di=138	?Ce=140	—	—	—	— — — —
9	(—)	—	—	—	—	—	—	
10	—	—	?Er=178	?La=180	Ta=182	W=184	—	Os=195, Ir=197, Pt=198, Au=199.
11	(Au=199)	Hg=200	Tl=204	Pb=207	Bi=208	—	—	
12	—	—	—	Th=231	—	U=240	—	— — — —

Ga=69.7 Ge=72.6

Mendeleev's **1871** periodic table

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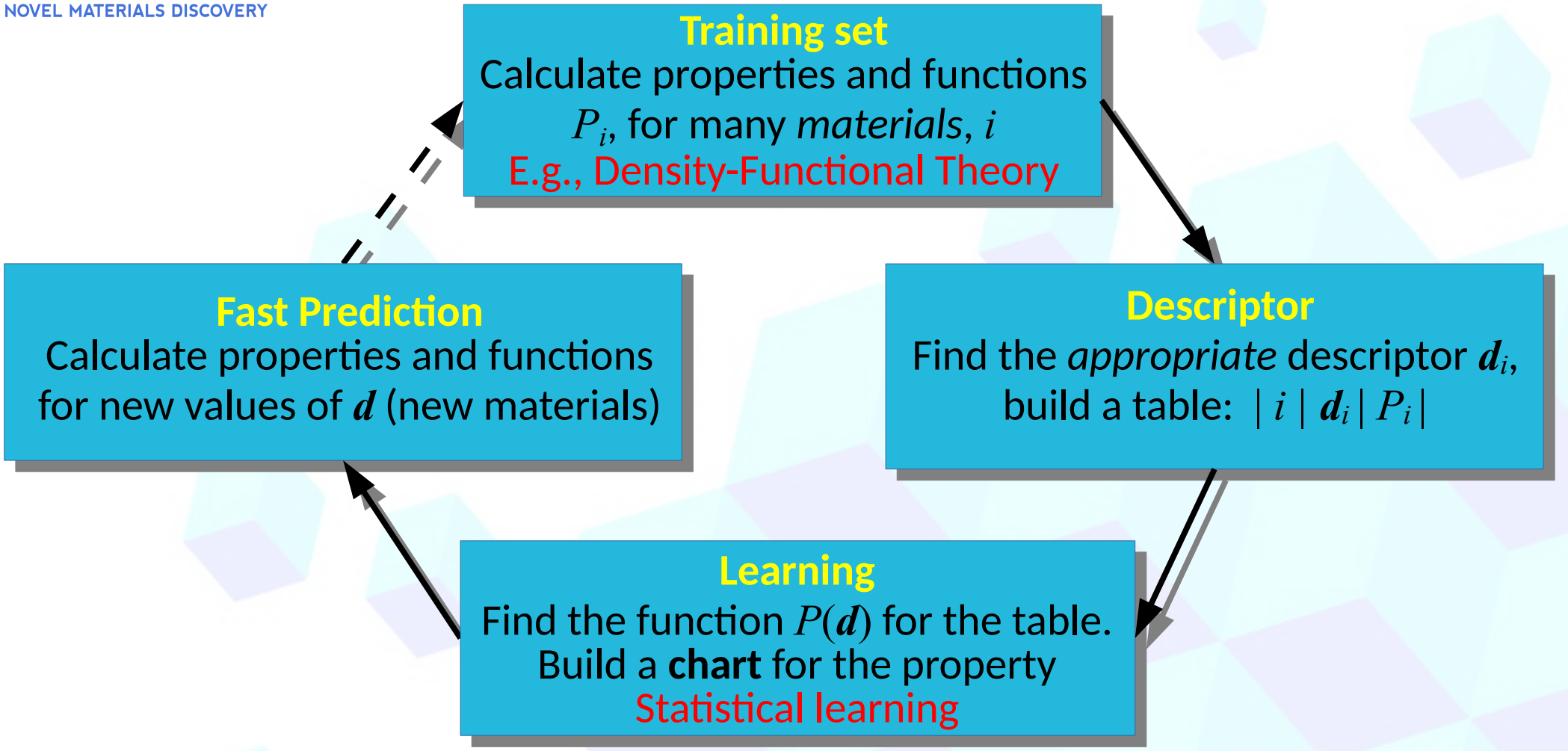
Data analytics: an ideal flow chart



Data analytics: an ideal flow chart

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Training set
Calculate properties and functions
P_i, for many *materials*, i
ory

$\{R_\mathrm{I}, Z_\mathrm{I}\} \rightarrow$ Hamiltonian

$\{R_\mathrm{I}\} \rightarrow$ Geometry
- translational, rotational, permutational invariant
- perhaps just lattice-decoration sensitive

$\{Z_\mathrm{I}\} \rightarrow$ Chemistry

C
fo

Descriptor
the *appropriate* descriptor $\boldsymbol{d}_i$,
build a table: $| i | \boldsymbol{d}_i | P_i |$

Learning
Find the function $P(\boldsymbol{d})$ for the table.
Build a **chart** for the property
Statistical learning

Learning/discovering maps of materials properties. A quantum many-body problem

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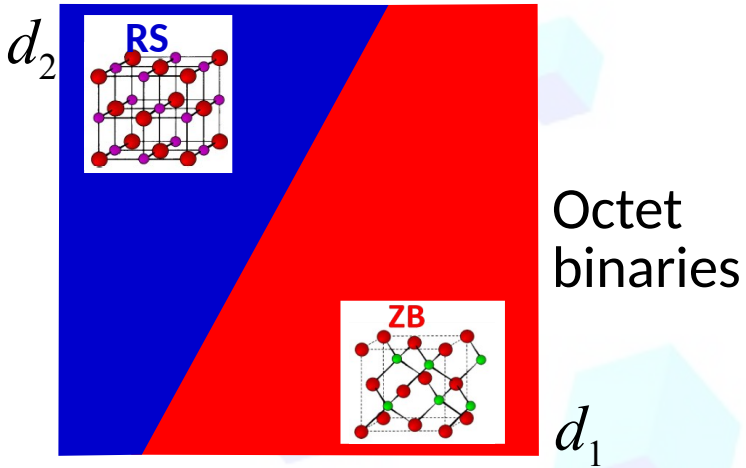
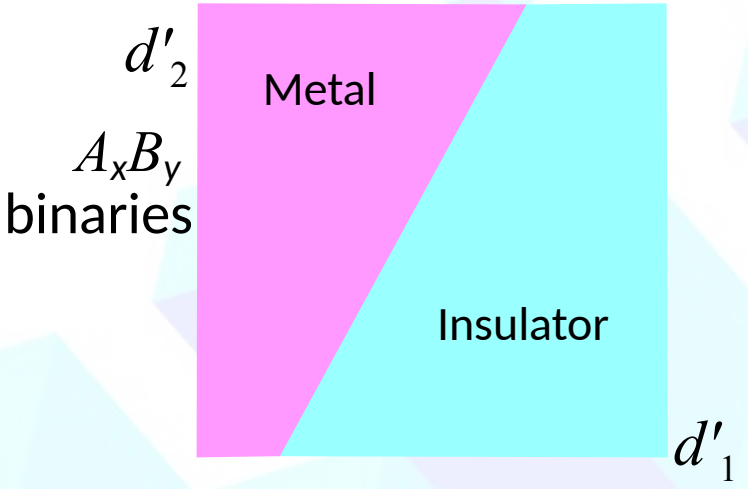
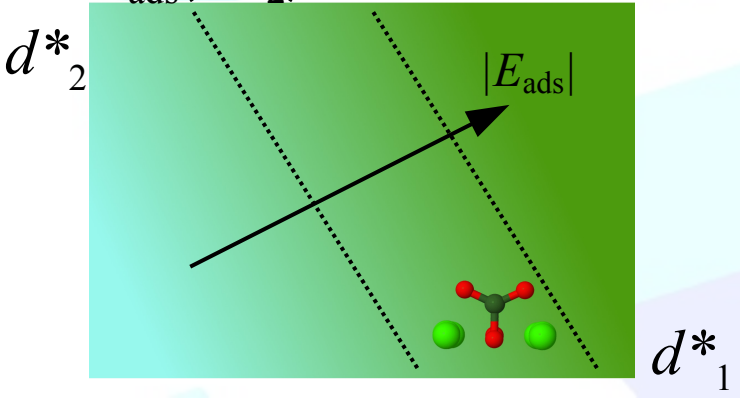


Octet binaries

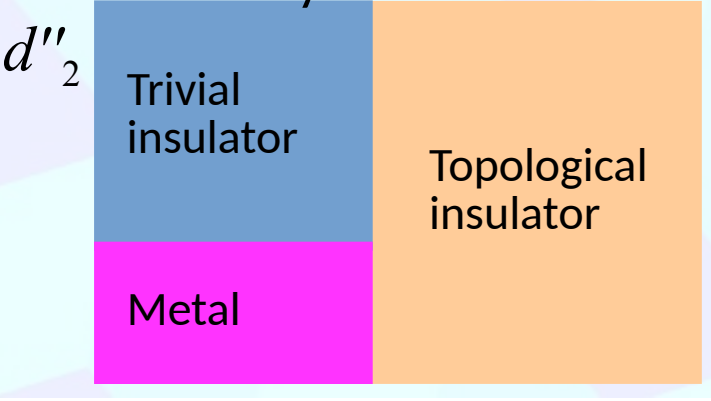


A_xB_y binaries

$E_{ads}(CO_2)$ on oxides



2D honeycomb materials



Learning/discovering maps of materials properties. A quantum many-body problem

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From the Hamiltonian of a physical system, in principle we can derive all properties (observables).
But in practice, the Hamiltonian is often not the starting point.

For instance, given a class of chemical compositions
(e.g., via prototype formula, such as ABX_3):

- what is the most stable crystal structure of each material in the class?
- which materials are metals / topological insulators / superconductors ?
- which material has the highest melting point?
- which materials has a surface optimal for catalysing some chemical reaction?

Compressed sensing: the quest for descriptors and predictive models

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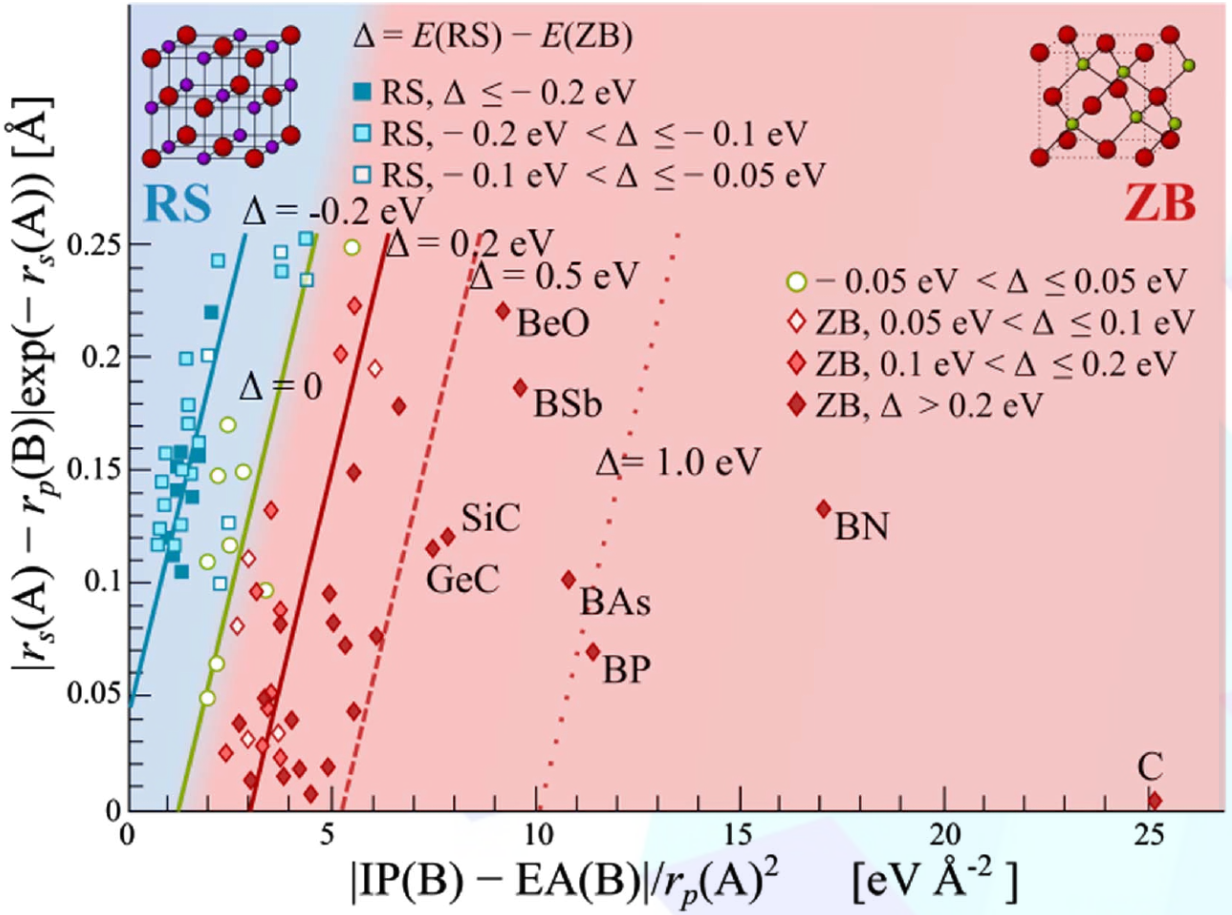


Structure map with compressed-sensing algorithm, starting from 7 atomic features

LMG *et al.*, PRL 2015, NJP 2017

Data analytics with compressed sensing

Compressed sensing

Aim: finding descriptors and learning predictive models

Ansatz:

$$\boldsymbol{P} = c_1\boldsymbol{d}_1 + c_2\boldsymbol{d}_2 + \ldots + c_n\boldsymbol{d}_n$$

$\boldsymbol{P}$: property of interest

$\boldsymbol{d}_1, \ldots \boldsymbol{d}_n$: features, i.e., (nonlinear) functions of *primary features* (EA, IP, ...)

$c_1, \ldots c_n$: unknown coefficients => as few as possible are *nonzero*

$$\underset{\boldsymbol{c}\in\mathbb{R}^M}{\operatorname{argmin}} \|\boldsymbol{P} - \boldsymbol{D}\boldsymbol{c}\|_2^2 + \lambda\|\boldsymbol{c}\|_0$$

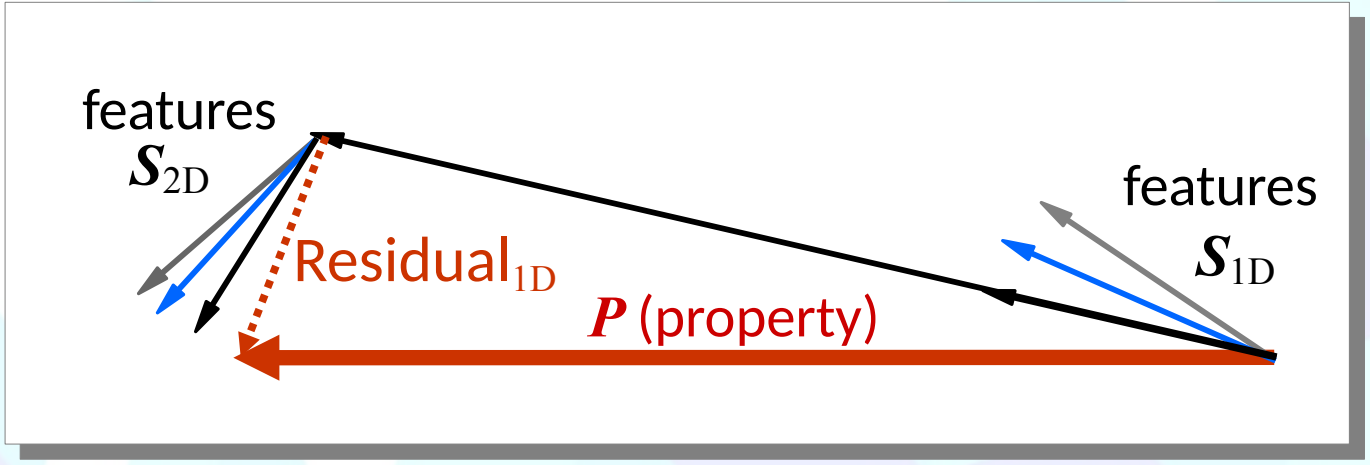
d_i: iterative construction with features and operators (+, ×, /, ², ...)

$$\frac{\mathrm{IP(B)} - \mathrm{EA(B)}}{r_p(\mathrm{A})^2}, \frac{|r_s(\mathrm{A}) - r_p(\mathrm{B})|}{\exp(r_s(\mathrm{A}))}$$

SISSO: sure independence screening plus sparsifying operator

NOVEL MATERIALS DISCOVERY

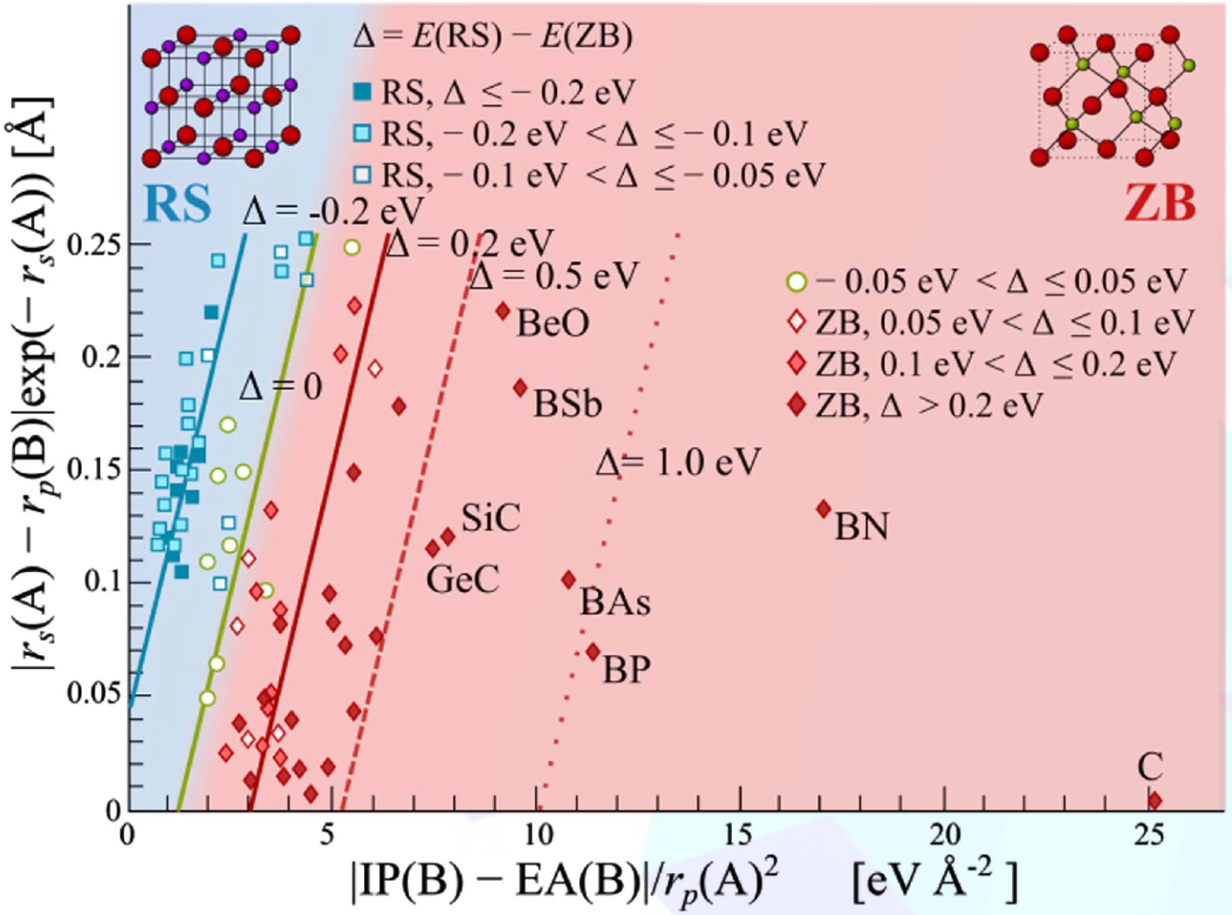
$$\underset{\boldsymbol{c}\in\mathbb{R}^M}{\operatorname{argmin}} \|\boldsymbol{P}-\boldsymbol{D}\boldsymbol{c}\|_2^2+\lambda\|\boldsymbol{c}\|_0$$



Ouyang, Curtarolo, Ahmetcik, Scheffler & LMG, PRM (2018) arXiv:1710.03319

Compressed sensing: the quest for descriptors and predictive models

NOVEL MATERIALS DISCOVERY



Structure map with compressed-sensing algorithm, starting from 7 atomic features

LMG *et al.*, PRL 2015, NJP 2017

One descriptor to rule them all: Multi-task learning

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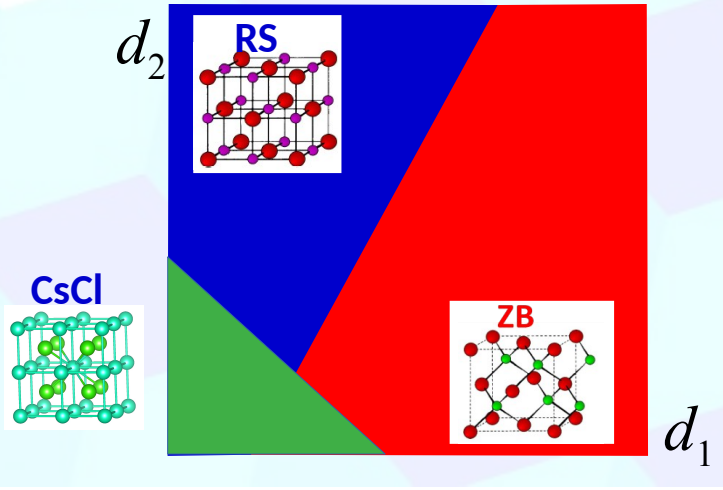
$$\{P^{(1)}, P^{(2)}, \ldots, P^{N^{\mathrm{T}}}\} \longrightarrow P^k = \boldsymbol{d} \cdot \boldsymbol{c}^k$$

$$\arg\min_{\boldsymbol{c}} \left(\|\boldsymbol{P} - \boldsymbol{D}\boldsymbol{c}\|_2^2 + \lambda \|\boldsymbol{c}\|_0 \right)$$

$$\arg\min_{\boldsymbol{C}} \sum_{k=1}^{N^{\mathrm{T}}} \frac{1}{N_k^{\mathrm{M}}} \left\| \boldsymbol{P}^k - \boldsymbol{D}^k \boldsymbol{C}^k \right\|_2^2 + \lambda \left\| \boldsymbol{C} \right\|_0$$

Application: multi-phase stability diagram
Properties: crystal-structure formation energies



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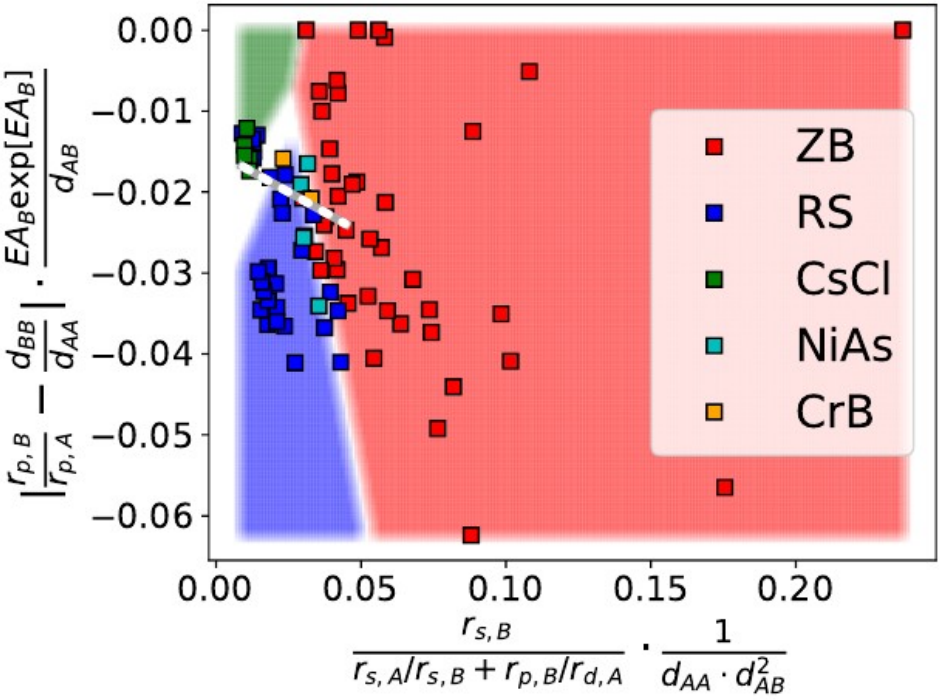
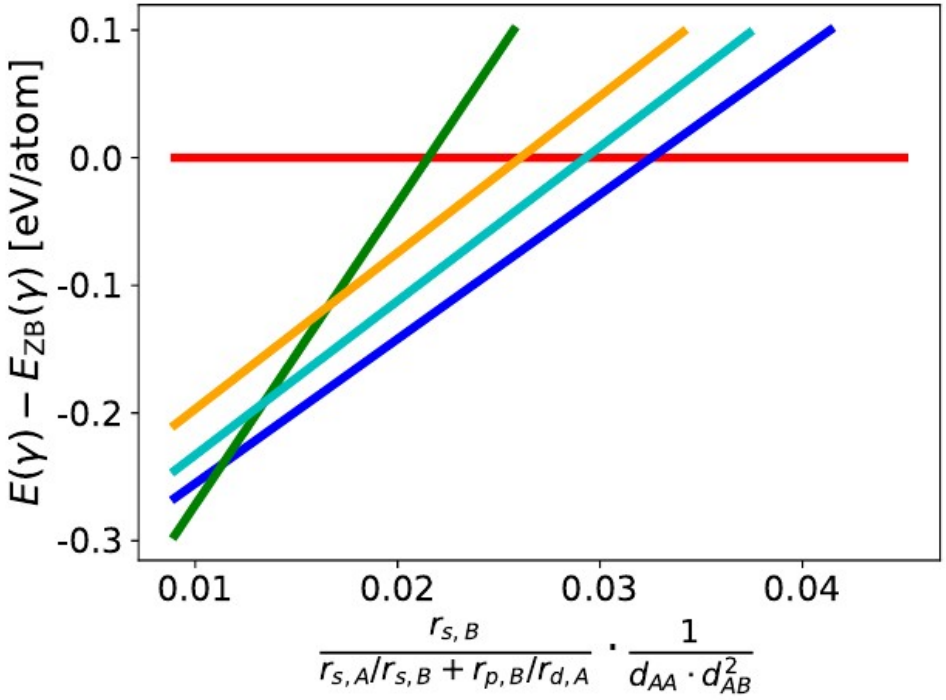
One descriptor to rule them all: Multi-task SISSO
Energy differences among 5 crystal structures.





Ouyang, Ahmetcik, Carbogno, Scheffler & LMG, arXiv:1901.00948

SISSO for classification

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$$\underset{\boldsymbol{c}\in\mathbb{R}^M}{\operatorname{argmin}}\left(\left\|\boldsymbol{P}-\boldsymbol{D}\boldsymbol{c}\right\|_2^2+\lambda\left\|\boldsymbol{c}\right\|_0\right)$$

New cost function to be minimized:
overlap of *convex* domains

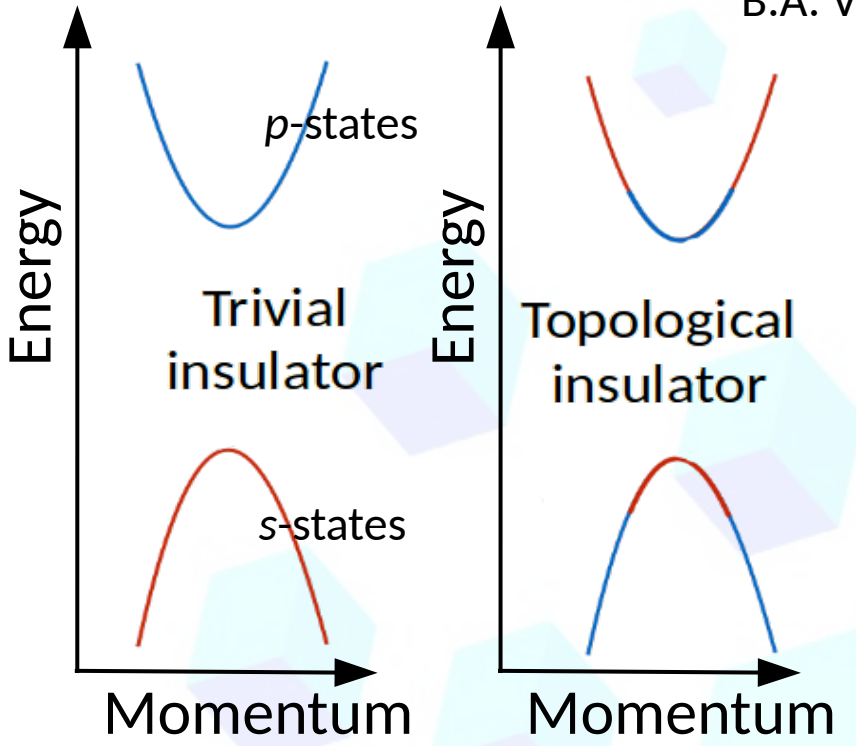
1. # points in the *convex* overlap domain
2. Area of the domain overlap
3. Distance between domains

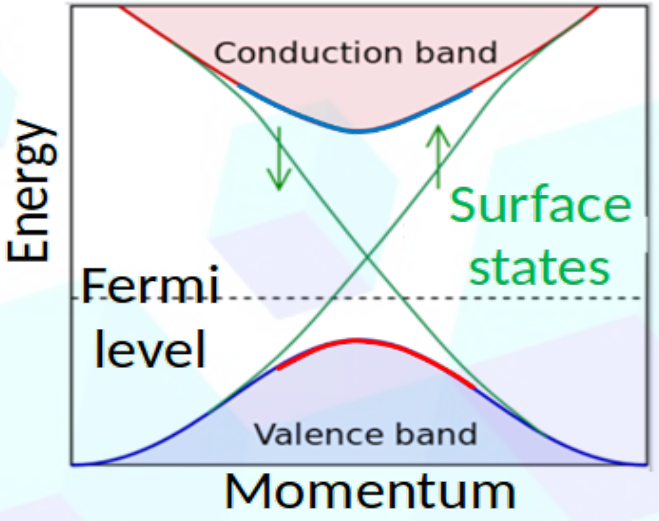
Good also for multi-categorical problems
(see A. F. Bialon *et al.*, Chem. Mater. **28**, 2550 (2016))

SISSO: predicting novel honeycomb (~2D) topological insulators

NOVEL MATERIALS DISCOVERY

B.A. Volkov, O.A. Pankratov, JETP Lett. **42**, 178 (1985)





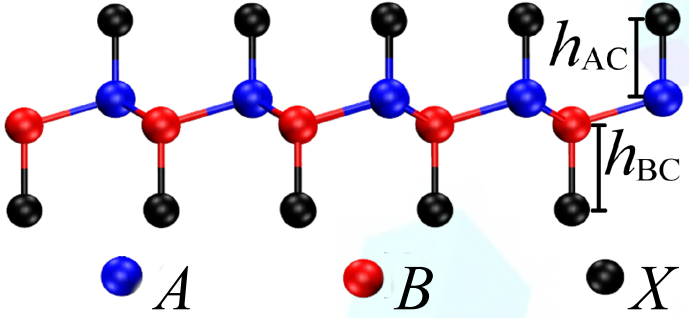
Triggered by:
spin-orbit coupling, alloying, strain, electric field

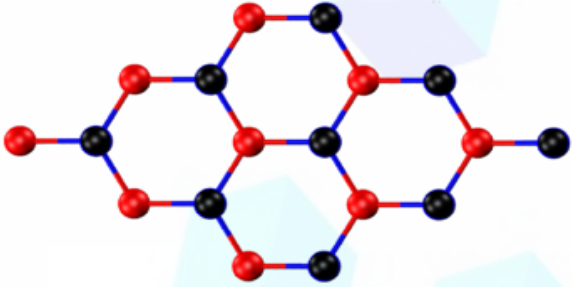
2D topological insulators:
No backscattering in edge states.
Characterized by a Z_2 topological index.

Promising materials in spintronics applications, e.g., quantum computing.

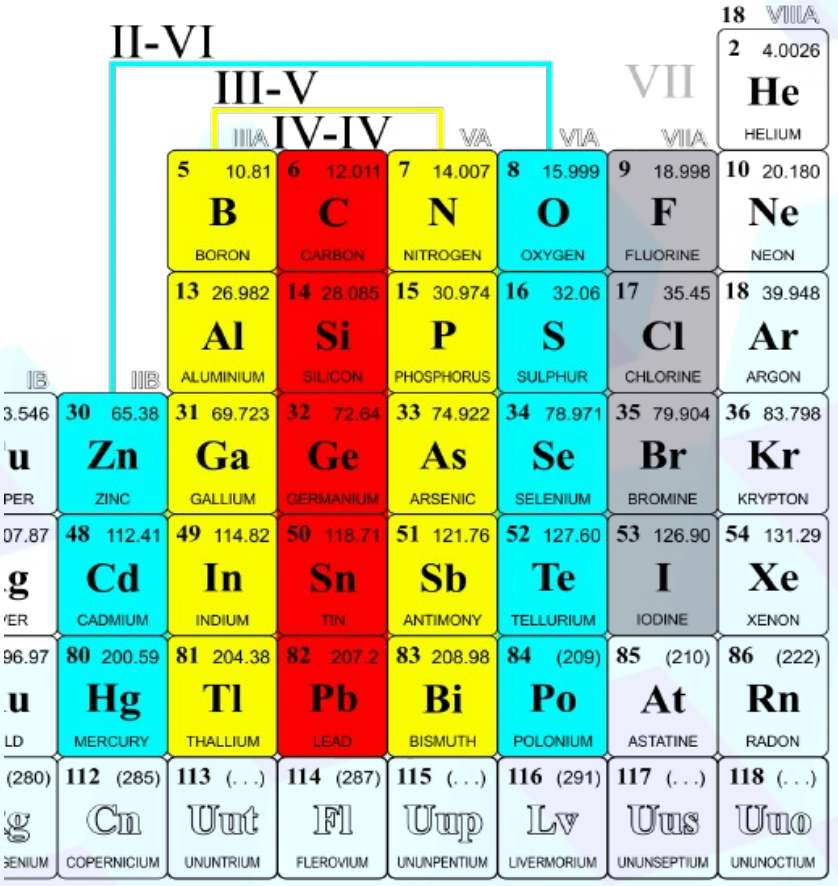
SISSO: predicting novel honeycomb (~2D) topological insulators

NOVEL MATERIALS DISCOVERY





A	II	III	IV
B	VI	V	IV
X	VII	VII	VII



Data source: high throughput DFT (FHI-aims, Carlos Mera Acosta)

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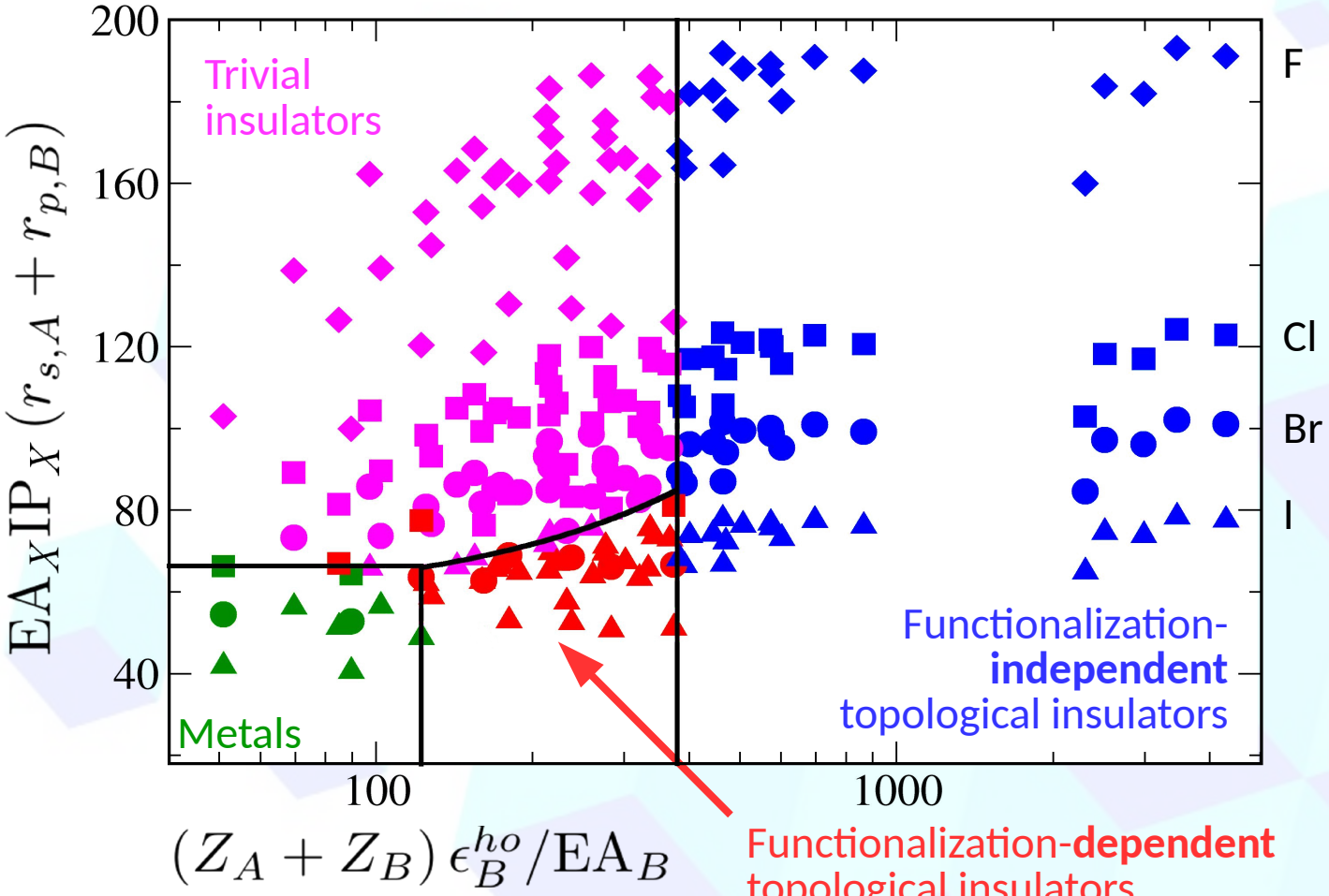
SISSO: predicting novel honeycomb (~2D) topological insulators



SISSO: predicting novel honeycomb (~2D) topological insulators

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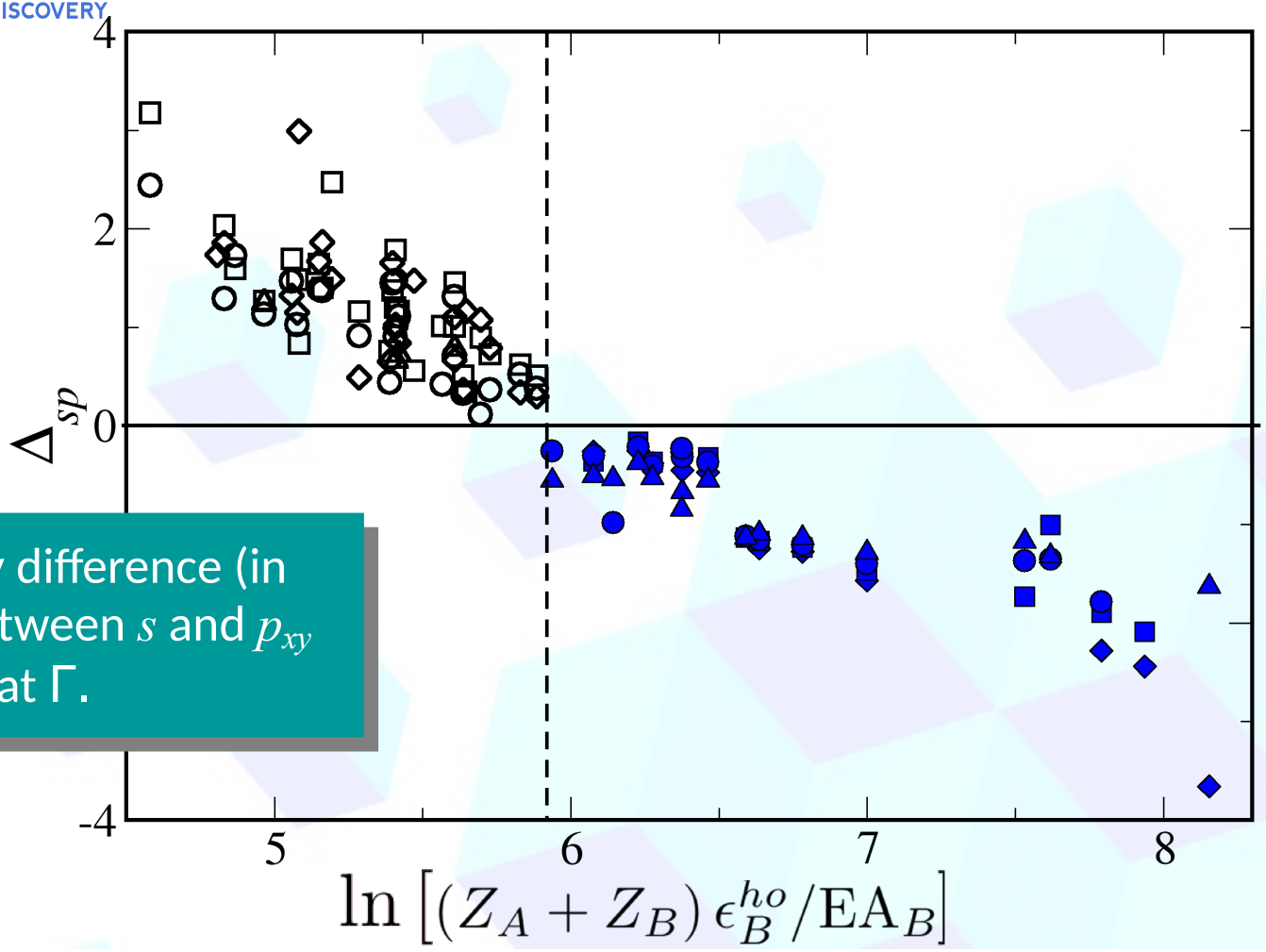

Energy difference (in eV) between s and p_{xy} states at Γ.

SISSO: predicting novel honeycomb (~2D) topological insulators

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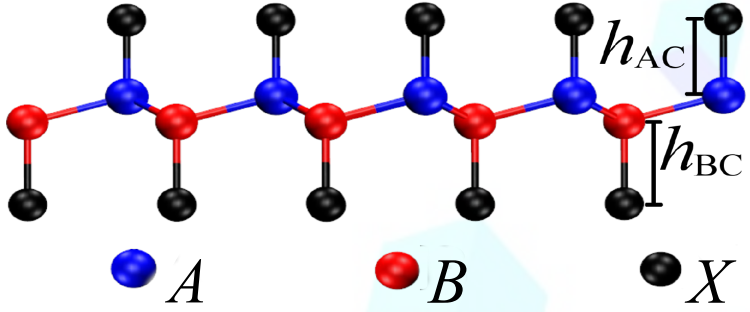
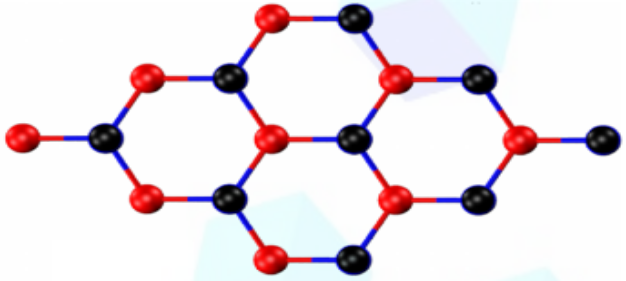
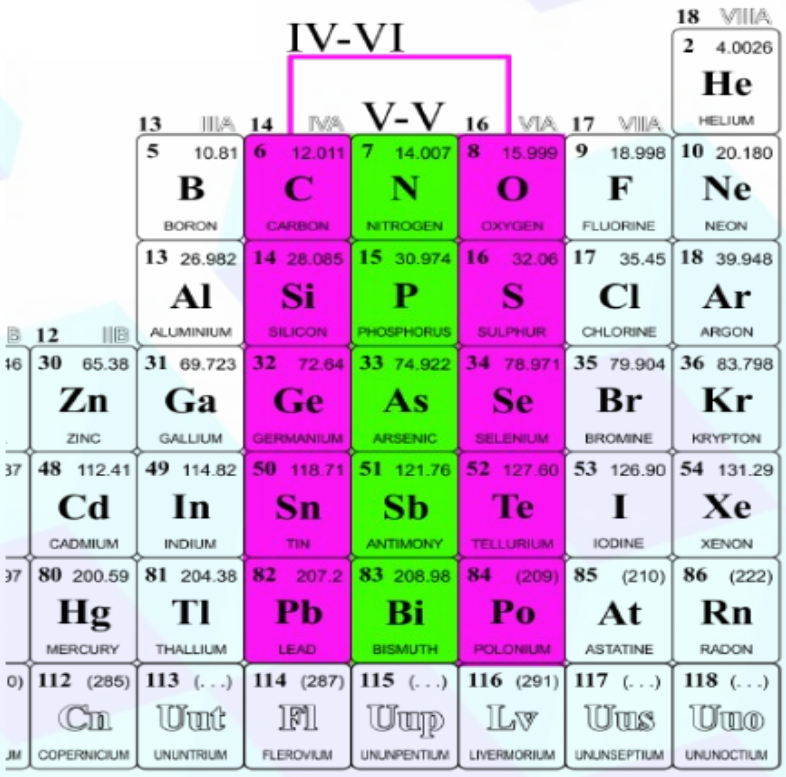




A	II	III	IV	IV V
B	VI	V	IV	VI V
X	VII	VII	VII	VI VI



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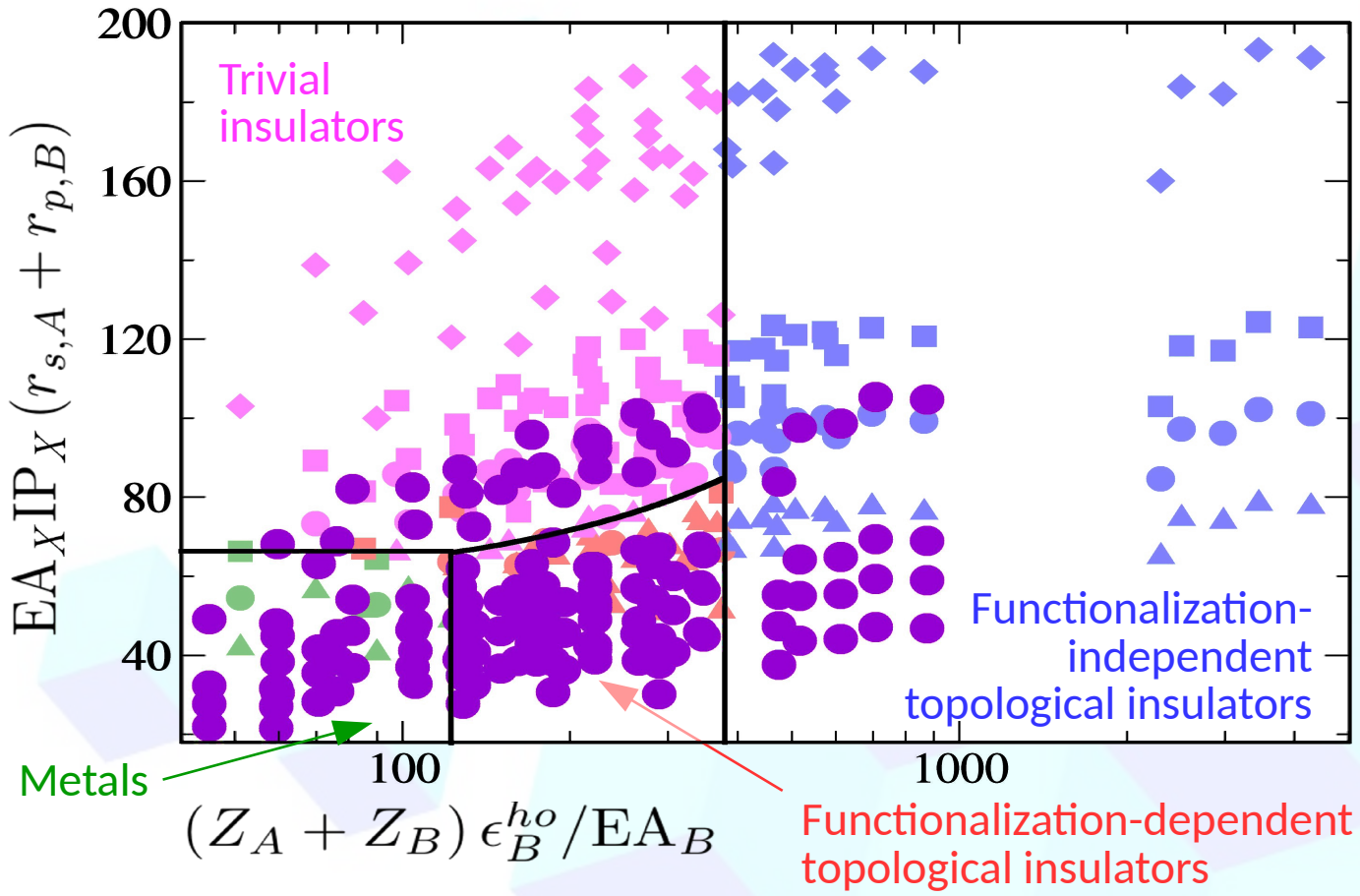
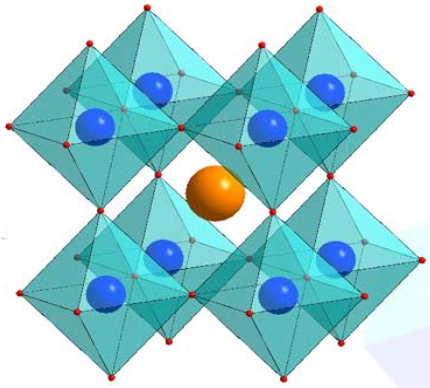


Mera Acosta, Ouyang, Fazzio, Scheffler, LMG & Carbogno, arXiv: 1805.10950a

Perovskites' stability: Improving on Goldschmidt Tolerance Factor

NOVEL MATERIALS DISCOVERY



ABX_3

$$t = \frac{r_A + r_X}{\sqrt{2}(r_B + r_X)}$$ → Ionic radius

Goldschmidt* stable perovskites: accuracy 74%

t = 0.825 t = 1.059 t

Bartel, Sutton, Goldsmith, Ouyang, Musgrave, LMG &Scheffler, Sci. Adv., in press. arXiv:1801.07700

Perovskites' stability: Improving on Goldschmidt Tolerance Factor

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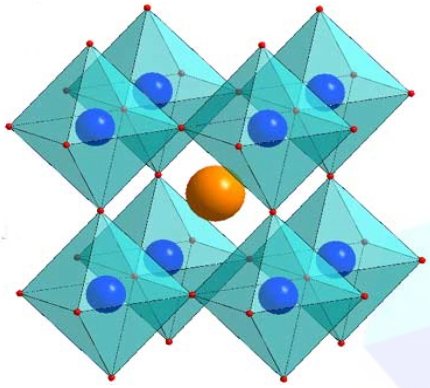

ABX_3

$$t = \frac{r_A + r_X}{\sqrt{2}(r_B + r_X)}$$

r_A, r_X: Ionic radius

$$\tau = \frac{r_X}{r_B} - n_A \left(n_A - \frac{r_A/r_B}{\ln(r_A/r_B)} \right)$$

n_A: Oxidation state

$\frac{r_X}{r_B}$: 1 / μ = Octahedral factor

Goldschmidt* stable perovskites: accuracy 74%

t = 0.825 t = 1.059 t

Our stable perovskites: accuracy 92%

τ = 4.18 τ

Bartel, Sutton, Goldsmith, Ouyang, Musgrave, LMG &Scheffler, Sci. Adv., in press. arXiv:1801.07700

Perovskites' stability: Improving on Goldschmidt Tolerance Factor

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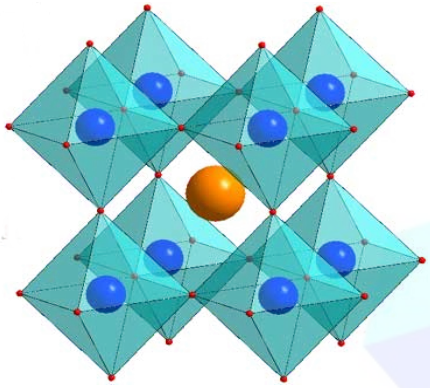

ABX_3

$$t = \frac{r_A + r_X}{\sqrt{2}(r_B + r_X)}$$

r_A, r_X, r_B → Ionic radius

n_A → Oxidation state

$$\tau = \frac{r_X}{r_B} - n_A\left(n_A - \frac{r_A/r_B}{\ln(r_A/r_B)}\right)$$

$\frac{r_X}{r_B}$ → 1 / μ = Octahedral factor

Goldschmidt* stable perovskites: accuracy 74%

t = 0.825 t = 1.059 t

Our stable perovskites: accuracy 99%

τ = 3.31 τ = 4.18 τ = 5.92 τ

Bartel, Sutton, Goldsmith, Ouyang, Musgrave, LMG &Scheffler, Sci. Adv., in press. arXiv:1801.07700

Perovskites' stability: Improving on Goldschmidt Tolerance Factor

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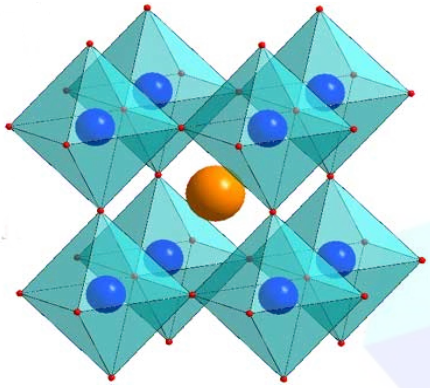


ABX_3

$$t = \frac{r_A + r_X}{\sqrt{2}(r_B + r_X)}$$ → Ionic radius

$$\tau = \frac{r_X}{r_B} - n_A \left(n_A - \frac{r_A/r_B}{\ln(r_A/r_B)} \right)$$ → Oxidation state

$\frac{r_X}{r_B}$ → 1 / μ = Octahedral factor

Goldschmidt* stable perovskites: accuracy 74%

t = 0.825 t = 1.059 t

Our stable perovskites: accuracy 100%

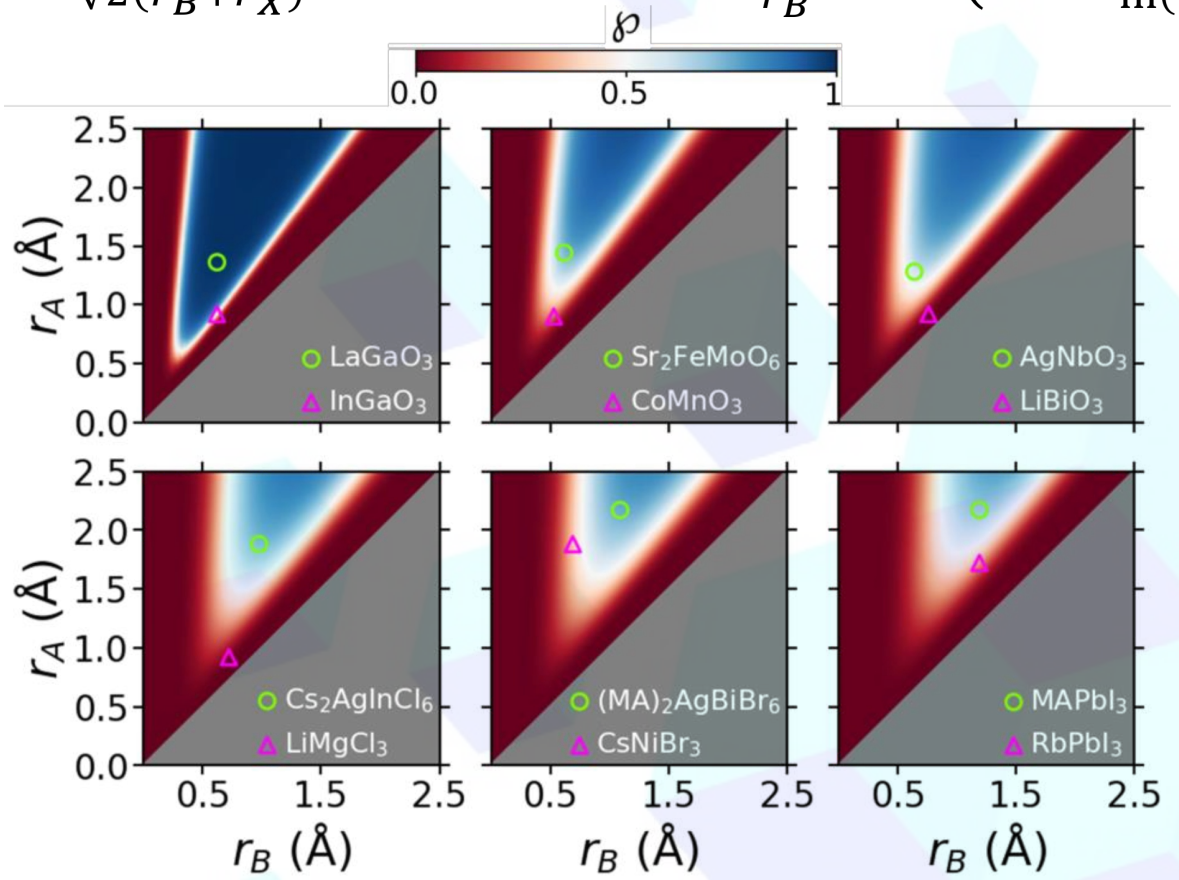
τ = 3.31 τ = 4.18 τ = 5.92 τ = 12.08 τ

Bartel, Sutton, Goldsmith, Ouyang, Musgrave, LMG &Scheffler, Sci. Adv., in press. arXiv:1801.07700

Perovskites' stability: Improving on Goldschmidt Tolerance Factor

NOVEL MATERIALS DISCOVERY

$$t = \frac{r_A + r_X}{\sqrt{2}(r_B + r_X)} \longrightarrow \tau = \frac{r_X}{r_B} - n_A\left(n_A - \frac{r_A/r_B}{\ln(r_A/r_B)}\right)$$



n_A

$X = O^{2-}$

$n_A = 1^+$

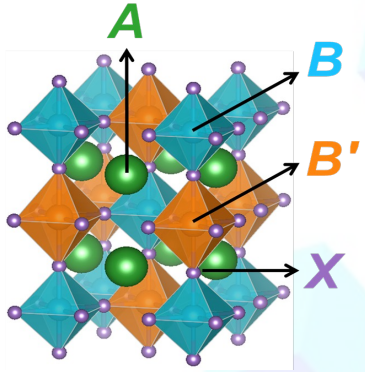
X

Perovskites' stability: Improving on Goldschmidt Tolerance Factor

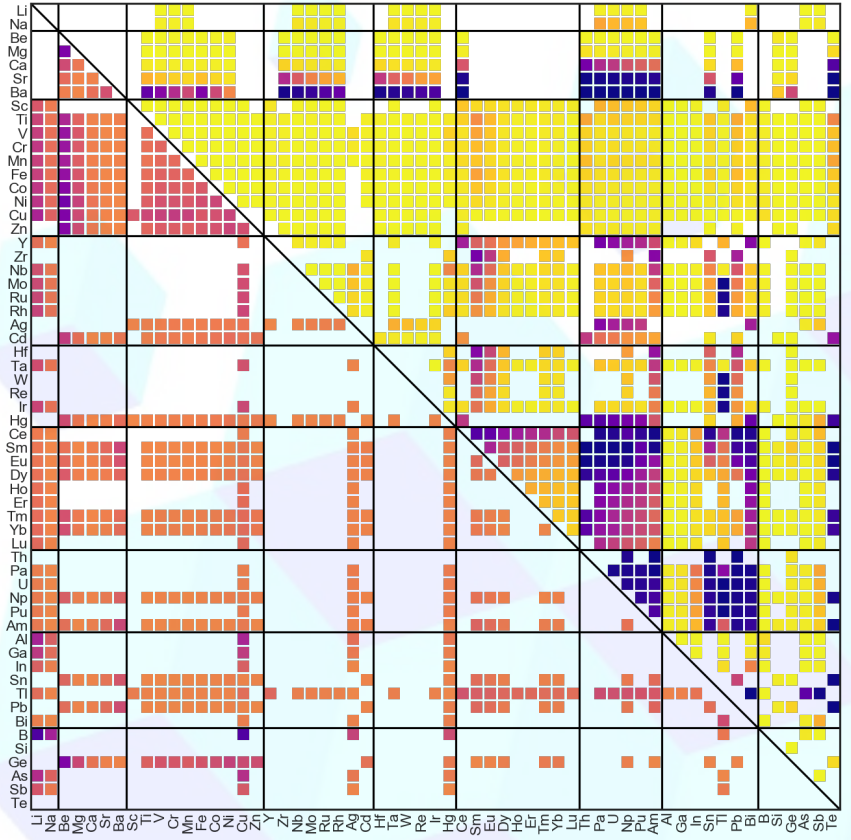
NOVEL MATERIALS DISCOVERY

$$t = \frac{r_A + r_X}{\sqrt{2}(r_B + r_X)} \longrightarrow \tau = \frac{r_X}{r_B} - n_A\left(n_A - \frac{r_A/r_B}{\ln(r_A/r_B)}\right)$$

Double perovskites

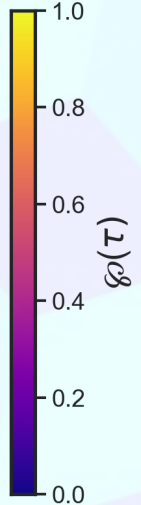


$r_B \rightarrow (r_B + r_{B'})/2$



$Cs_2BB'Cl_6$

$La_2BB'O_6$



… and more

Continuous property

Adsorption energy and OCO angle of adsorbed CO_2 on metal-oxide surfaces

Adsorption energy of O on metal-oxide surfaces

Adsorption energy of metal atoms on metal-alloys surfaces
Features: atoms (of the surface) and pristine surface

Classification

Tetradymite 5-component 3d topological insulators (vs trivial insulators)

Crowd sourcing data-driven materials science: nomad-coe.eu/outreach/nomad-kaggle-2018

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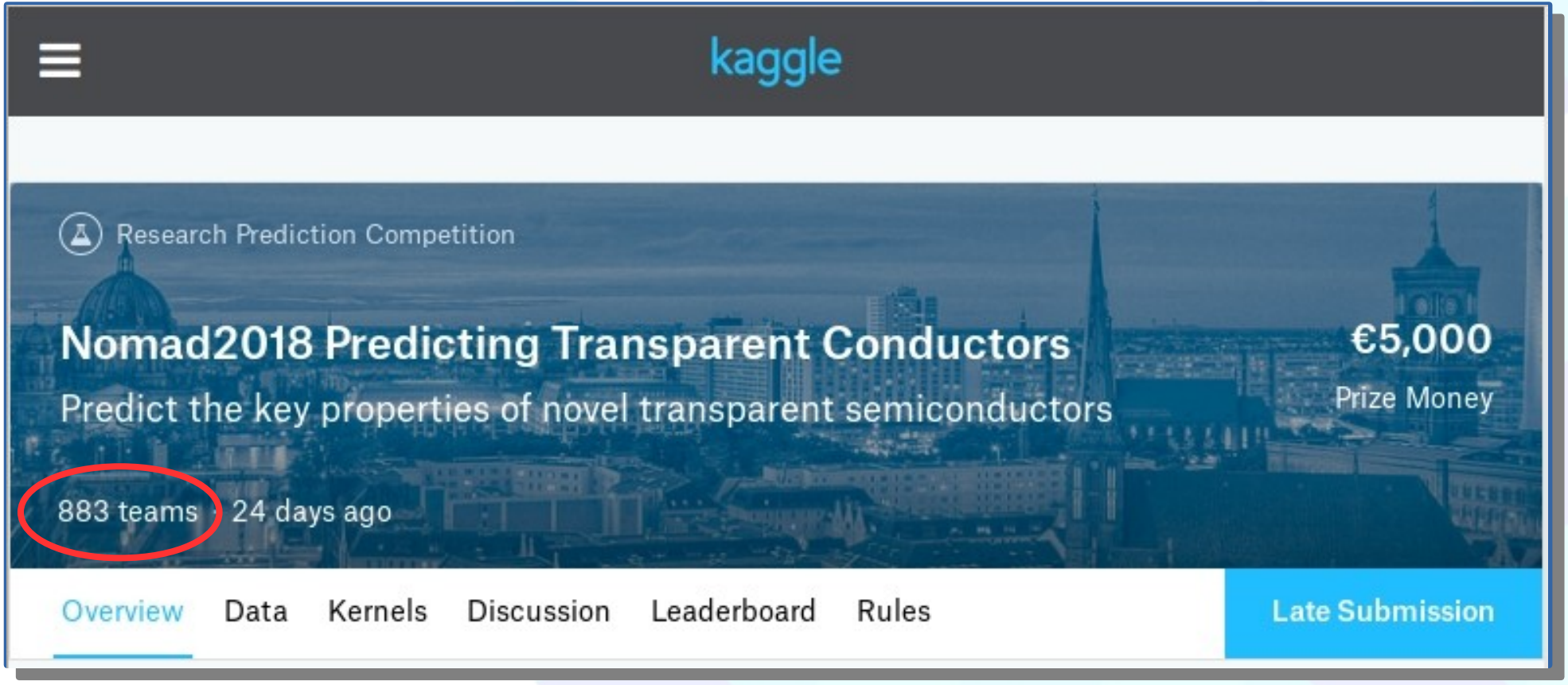

Crowd sourcing data-driven materials science: nomad-coe.eu/outreach/nomad-kaggle-2018

NOVEL MATERIALS DISCOVERY

- Materials class: $Al_xGa_yIn_zO_3$, $x + y + z = 3$, in 6 crystal prototypes (C2/m (12), Pna21 (33), R-3c (167), p63/mmc (194), Ia-3 (206), and Fd-3m, up to 96 atoms per unit cell
- Properties: Formation energy and band gap
- **Input: *Vegard's-law* lattice vectors and coordinates**
- ~3000 data points (2400 training + 600 validation set) calculated via PBE, by FHI-aims + Christopher Sutton

Crowd sourcing data-driven materials science: nomad-coe.eu/outreach/nomad-kaggle-2018

NOVEL MATERIALS DISCOVERY

Prediction accuracy	
Formation energy:	~20 meV/cation
Band gap:	~80 meV

1st **Takenori Yamamoto (Tony Y.)**
Descriptor: Crystal-graph *n*-grams
ML method: Kernel ridge regression

2nd **Dr. Yury Lysogorskiy**
Descriptor: 7000 average and local-order scalar features
ML method: Gradient boosting regression trees

3rd **Lars Blumenthal**
Descriptor: based on Smooth Overlap of Atomic Positions (SOAP)
ML method: Neural network

(Average) SOAP: S De, AP Bartók, G Csányi, M Ceriotti Phys. Chem. Chem. Phys. 18, 13754 (2016)
Sutton, LMG, Yamamoto, Lysogorskiy, Blumenthal, Hammerschmidt, Golebiowski, Liu, Ziletti, Scheffler arXiv:1812.00085

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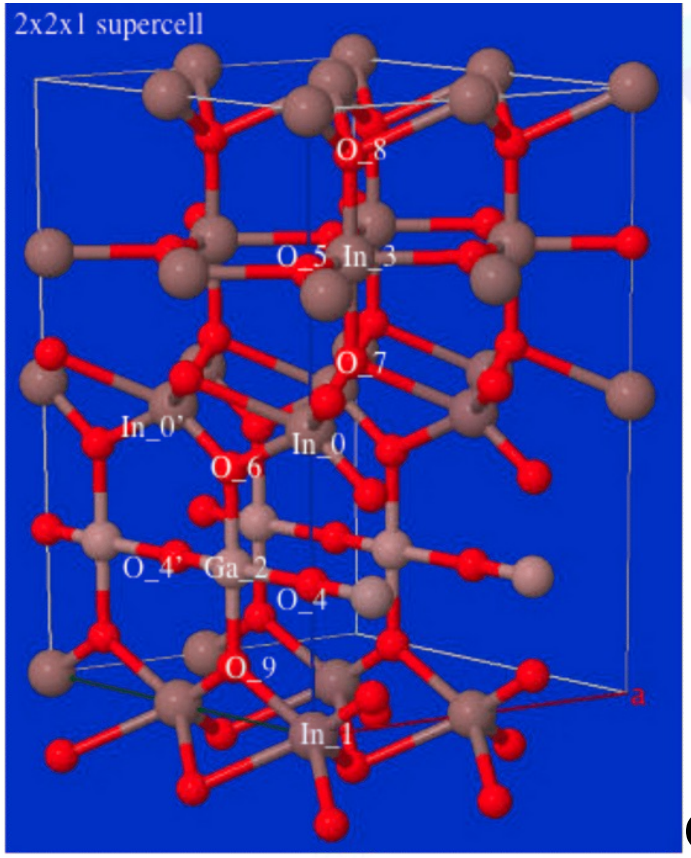
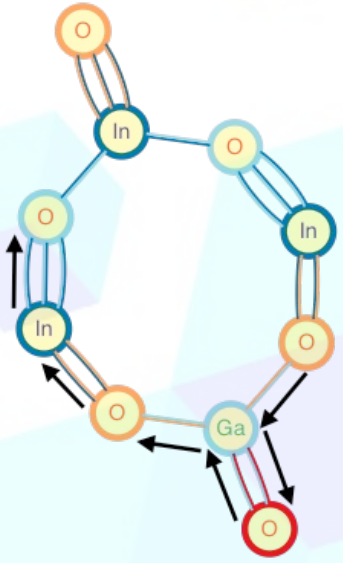


$GaIn_3O_6$

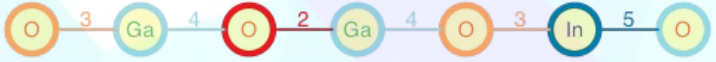
n-grams

Crystal Graph



Coordination Number

Path Graph



Sequence of N-gram Items

Sutton, LMG, Yamamoto, Lysogorskiy, Blumenthal, Hammerschmidt, Golebiowski, Liu, Ziletti, Scheffler arXiv:1812.00085

Crowd sourcing data-driven materials science: The importance of the descriptor

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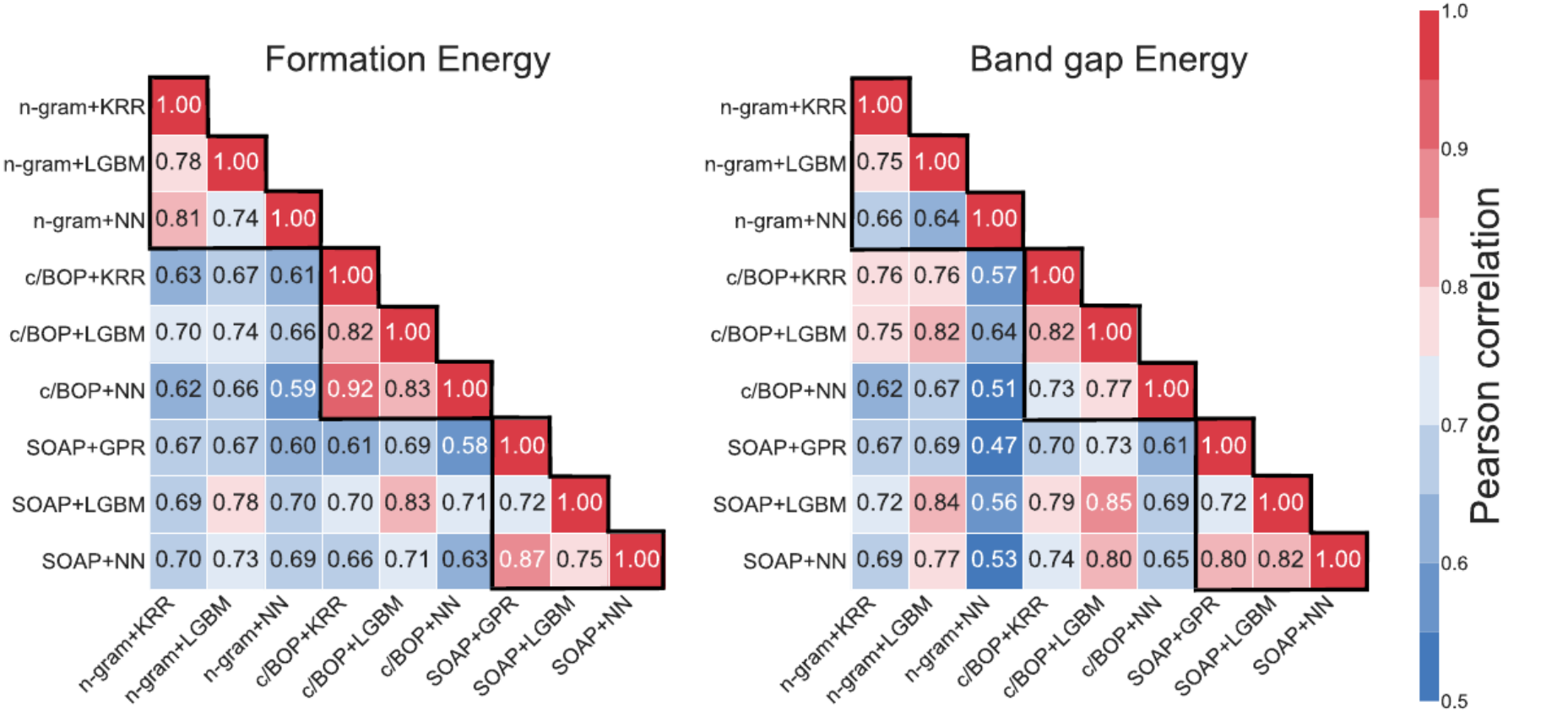

Sutton, LMG, Yamamoto, Lysogorskiy, Blumenthal, Hammerschmidt, Golebiowski, Liu, Ziletti, Scheffler arXiv:1812.00085

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The Novel Materials Discovery (NOMAD) Laboratory maintains the largest Repository, for input and output files of all important computational materials science codes.

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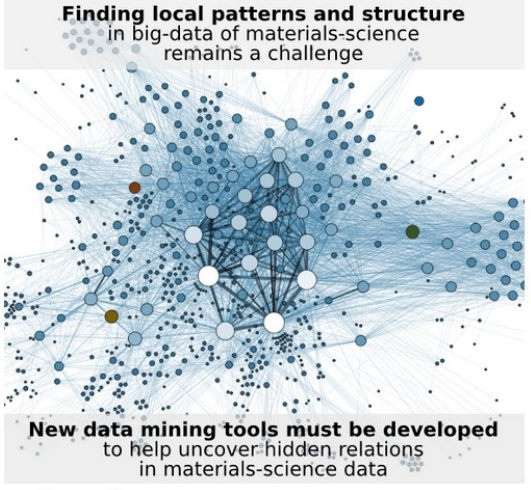

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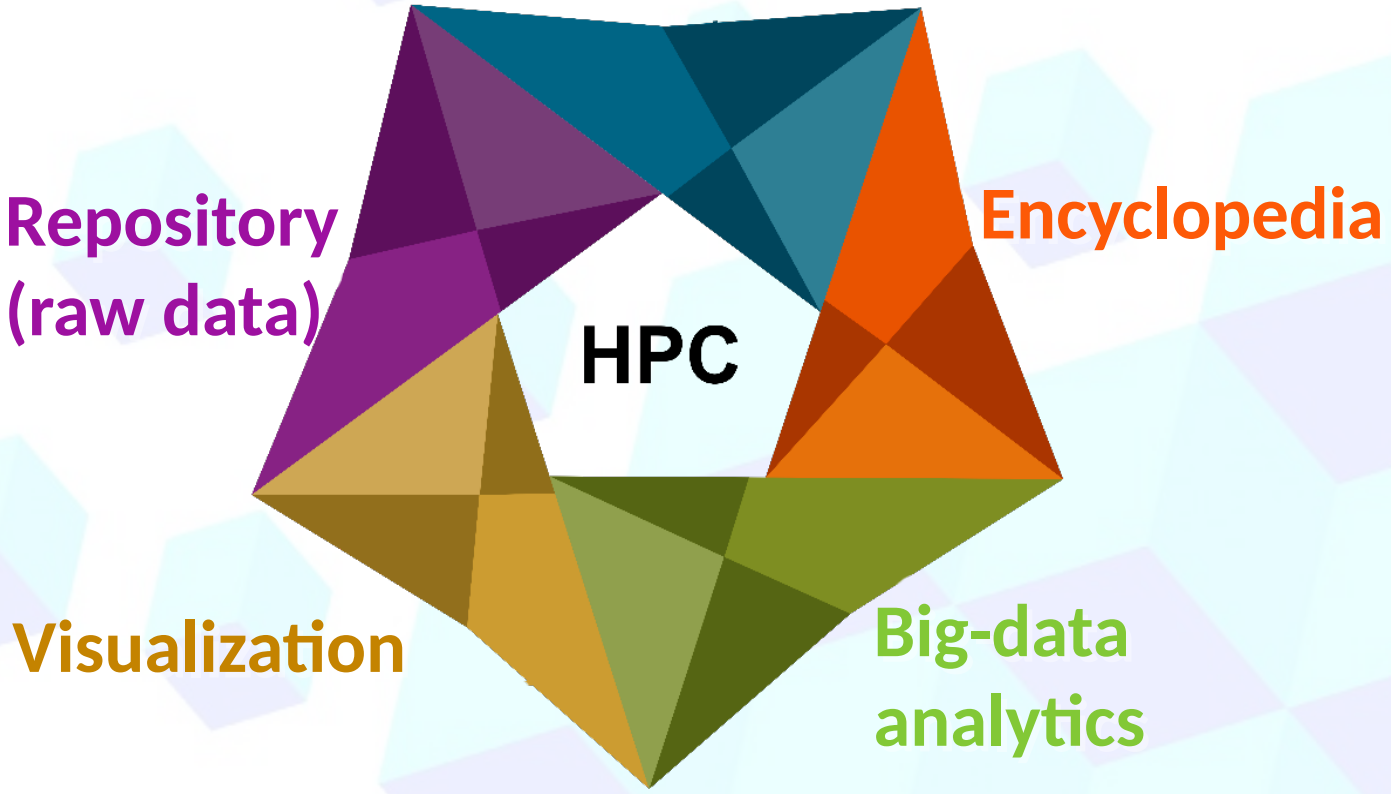

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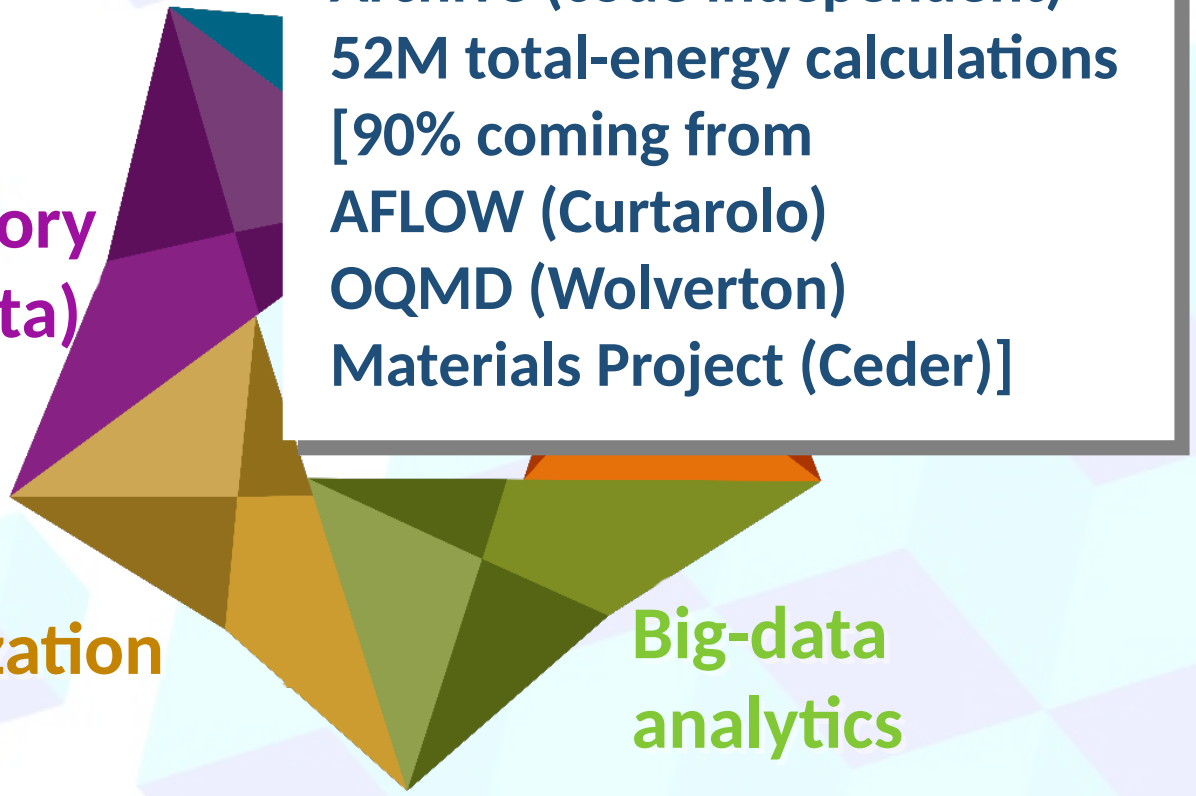

Archive (code independent)
52M total-energy calculations
[90% coming from
AFLOW (Curtarolo)
OQMD (Wolverton)
Materials Project (Ceder)]

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NOVEL MATERIALS DISCOVERY

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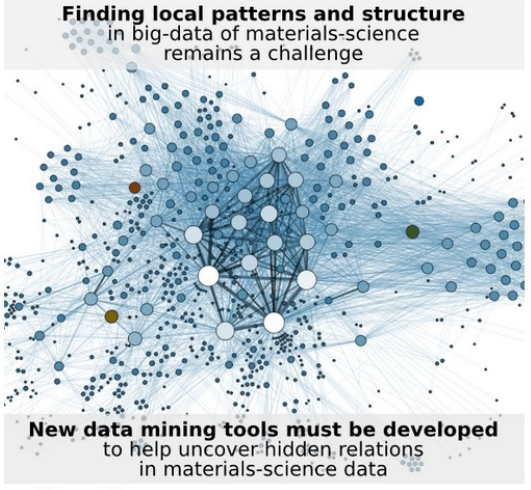

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NOVEL MATERIALS DISCOVERY

Materials property prediction

Predicting the metal-insulator classification of elements and binary systems

Prediction of topological quantum phase transitions

NOMAD Analytics Toolkit

– Prediction of topological quantum phase transitions

created by: Carlos Mera Acosta[1,2], Emre Ahmetcik [1], Adalberto Fazzio[2], Luca Ghiringhelli[1], and Matthias Scheffler[1]

[1] Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, D-14195 Berlin, Germany
[2] Brazilian Nanotechnology National Laboratory, Campinas, SP, Brazil

v1.0.0

[Last updated: November 9, 2017]

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Perovskites
Christopher J. Bartel, Christopher Sutton, Bryan R. Goldsmith, Runhai Ouyang, Charles B. Musgrave

NOMAD-Kaggle competition
Christopher Sutton, Angelo Ziletti, Xiangyue Liu

NOMAD PIs
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